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Coherent potential approach to exchange-induced band splitting in diluted magnetic semiconductors under a saturating magnetic field

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Abstract

Applying the coherent potential approximation (CPA) to a model which describes magnetic and chemical disorder in an $A^{II}_{1-x}Mn_xB^{VI}$-type diluted magnetic semiconductor (DMS) with a strong applied magnetic field, we calculate the band-edge energy shift as a function of the Mn concentration (x). The effects of the band offset and exchange interaction on the extended carrier state in a DMS are studied systematically. The apparent enhancement of the p–d exchange interaction which is observed in $Cd_{1-x}Mn_xS$ is explained well as a multiple-scattering effect which is significant for small x in disordered systems. The dominant origin is not a large attractive chemical potential at the Mn site, but a large exchange energy relative to the bandwidth.

The virtual-crystal approximation (VCA) is widely accepted for describing the field-induced exchange splitting of extended states in $A^{II}_{1-x}Mn_xB^{VI}$-type diluted magnetic semiconductors (DMSs). The VCA is a first-order perturbation theory approximation with respect to the sp–d exchange interaction between the sp-like band carrier and the localized d spin at the Mn site. In the standard VCA, first the molecular-field approximation (MFA) is applied to take the thermal average over the magnetic moment on substitutional magnetic ions, then the VCA is applied for the disordered alloy in which the magnetic moment is replaced beforehand by the thermally averaged one. Thus, according to the VCA with the MFA, the energy splitting between σ^+ and σ^- A excitons in a DMS is given as [1, 2]

$$\Delta E = N_0(\alpha - \beta)x\langle S_z\rangle \tag{1}$$

where $N_0\alpha$ and $N_0\beta$ are the exchange constants for conduction electrons and valence electrons, respectively, and $\langle S_z\rangle$ is the thermally averaged value of the d spin operator S_z on Mn^{2+} ions. The values of $N_0\alpha$ and $N_0\beta$ estimated using equation (1) for Mn-based wide-gap DMSs lie in the ranges $0.18 < N_0\alpha < 0.26$ eV and $-1.4 < N_0\beta < -0.9$ eV, except for $Cd_{1-x}Mn_xS$ [2]. $Cd_{1-x}Mn_xS$ is distinguishable from other DMSs because the apparent value of $|N_0\beta|$ for

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$Cd_{1-x}Mn_xS$ is considerably larger than the $|N_0\beta|$ values of other DMSs and varies with the Mn concentration x [3]. The experimentally deduced values of $N_0\beta$ for $Cd_{1-x}Mn_xS$ are reported to be $(x, N_0\beta) = (0.001, -3.3\text{ eV})$, $(0.005, -2.86\text{ eV})$, $(0.014, -2.09\text{ eV})$ (reference [4]), $(0.0015, -3.4\text{ eV})$, $(0.0055, -2.95\text{ eV})$ (reference [5]), $(0.005, -2.7\pm0.4\text{ eV})$ (reference [6]), and $(0.013, -1.8\text{ eV})$ (reference [7]).

A pioneering study on the abnormal x-dependence of $N_0\beta$ observed in $Cd_{1-x}Mn_xS$ was performed by Benoit à la Guillaume *et al* [8]. Assuming a large attractive potential due to the valence band offset ($E_M = -0.5$ eV) for a hole in $Cd_{1-x}Mn_xS$, Benoit à la Guillaume *et al* ascribed the abnormal x-dependence of the spin splitting to a large (nearly binding) exchange potential assisted by a valence band offset of the Mn ion. However, recent studies have revealed that E_M has a small positive value ($E_M = 0.09$ eV) for $Cd_{1-x}Mn_xS$ [9, 10]. Therefore, the effect of E_M on the exchange-induced band splitting must be reinvestigated. Later, Tworzydlo formulated the diluted alloy approach for a nearly binding substitutional potential of magnetic ions, taking the disorder into account [11, 12]. However, the range of application of Tworzydlo's theory was not clarified.

The aim of our study is to achieve a unified understanding of the effect of the exchange interaction between a carrier (electron or hole) and magnetic ions in DMSs. In a previous paper [13], we proposed a model for the extended state of a carrier in a DMS, in which magnetic and chemical disorder are taken into consideration, and applied the coherent potential approximation (CPA) to the model for paramagnetic states to explain the abnormal x-dependence of the band-gap energy referred to as bowing. In the present work, we apply the CPA to the model with a strong applied magnetic field, in order to explain the abnormal x-dependence of the exchange integral ($N_0\beta$) observed for $Cd_{1-x}Mn_xS$.

When a carrier moves in a disordered system of binary solid solutions, it is subjected to a local potential E_A or E_B depending on whether the atom therein is an A atom or a B atom. The CPA is a superior mean-field theory that is applicable for describing the electronic properties of binary substitutional alloys within the single-site approximation [14–16]. In the CPA, the disordered potential is considered in terms of the effective-medium Σ, called the coherent potential or self-energy; $\Sigma \equiv \Sigma(\omega)$ is an energy- (ω-) dependent complex potential which is decided such that the effective scattering of a carrier at the chosen site embedded in the effective medium is zero, on average. The condition is given by

$$(1-x)\frac{E_A - \Sigma}{1-(E_A-\Sigma)F} + x\frac{E_B-\Sigma}{1-(E_B-\Sigma)F} = 0. \tag{2}$$

Here, $(1-x)$ and x are the mole fractions of A and B atoms, respectively. Hereafter, we set $E_A \equiv 0$ as the origin of the energy.

$F \equiv F(\omega)$ is the diagonal matrix element of the reference Green's function in the Wannier representation. Introducing the model density of states in the semicircular form with a half-bandwidth Δ as an undisturbed density of states (i.e., for $E_B = E_A = 0$), F is calculated from

$$F \equiv F(\omega) = \frac{2}{\pi\Delta}\int_{-\Delta}^{\Delta} d\varepsilon \sqrt{1-\left(\frac{\varepsilon}{\Delta}\right)^2}\frac{1}{\omega-\varepsilon-\Sigma}. \tag{3}$$

Equation (3) leads to the simple relation [13]

$$\Sigma = \omega - \frac{\Delta^2}{4}F - F^{-1}.$$

Inserting this relation into equation (2), the CPA condition, we obtain the cubic equation for $F\Delta \equiv F(\omega)\Delta$, namely

$$(F\Delta)^3 + 4\left(\frac{E_B - 2\omega}{\Delta}\right)(F\Delta)^2 + 4\left\{1 + \frac{4\omega(\omega - E_B)}{\Delta^2}\right\}(F\Delta) + 16\left\{\frac{(1-x)E_B - \omega}{\Delta}\right\} = 0. \tag{4}$$

Using the complex-conjugate root of equation (4), the density of states $D(\omega)$ is calculated from

$$D(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,F(\omega).$$

Thus, the condition that the value of the discriminant of equation (4) should vanish leads to the condition for the band-edge energy, ω_b [15]:

$$\left(\frac{\omega_b}{\Delta}\right)^4 + A\left(\frac{\omega_b}{\Delta}\right)^3 + B\left(\frac{\omega_b}{\Delta}\right)^2 + C\left(\frac{\omega_b}{\Delta}\right) + D = 0 \tag{5}$$

with

$$A = -\frac{1}{2}\left(\frac{\Delta}{E_\mathrm{B}}\right)\left\{(1-2x) + 4\left(\frac{E_\mathrm{B}}{\Delta}\right)^2\right\} \tag{6a}$$

$$B = \frac{1}{16}\left(\frac{\Delta}{E_\mathrm{B}}\right)^2\left\{16\left(\frac{E_\mathrm{B}}{\Delta}\right)^4 - 8(3x+1)\left(\frac{E_\mathrm{B}}{\Delta}\right)^2 + 1\right\} \tag{6b}$$

$$C = \frac{1}{16}\left(\frac{\Delta}{E_\mathrm{B}}\right)\left\{8(4-3x)\left(\frac{E_\mathrm{B}}{\Delta}\right)^2 + 2(4-9x)\right\} \tag{6c}$$

$$D = -\frac{1}{16}\left(\frac{\Delta}{E_\mathrm{B}}\right)^2\left\{16(1-x)\left(\frac{E_\mathrm{B}}{\Delta}\right)^4 + (27x^2 - 36x + 8)\left(\frac{E_\mathrm{B}}{\Delta}\right)^2 + 1\right\}. \tag{6d}$$

For the energy of the bottom of the band, ω_b, the energy shift is given by $\Sigma_b \equiv \omega_b + \Delta$. In order to clarify the analytic features of Σ_b, it is more convenient to make the approximation $\omega_b = -\Delta + \Sigma(\omega_b)$ [13], which yields $F(\omega_b)\Delta = -2$. Substituting $F(\omega_b)\Delta = -2$ into equation (2), we obtain the energy shift in the lowest band edge, i.e. real Σ_b ($\equiv\omega_b+\Delta = \Sigma(\omega_b)$):

$$\frac{\Sigma_b}{\Delta} = \frac{1}{2}\left\{\left(\frac{1}{2} + \frac{E_B}{\Delta}\right) - \sqrt{\left(\frac{1}{2} + \frac{E_B}{\Delta}\right)^2 - 2x\left(\frac{E_B}{\Delta}\right)}\right\}. \tag{7}$$

The exact Σ_b ($\equiv\omega_b + \Delta$) is obtained for an ω_b that is one of the real solutions for equation (5) with equation (6), while the approximate one is given by equation (7). It has been confirmed that the difference between the exact Σ_b and the approximate one (equation (7)) is evaluated to be within 1%.

Now, applying the present approximation to the previously proposed model [13] with a strong applied magnetic field, we explain the apparent enhancement in $N_0\beta$ observed in $Cd_{1-x}Mn_xS$ when $x \to 0$. When the applied magnetic field is saturating, the potential to which a hole with $\uparrow$ spin ($\downarrow$ spin) is subjected at the Mn site is regarded as $E_\mathrm{B} = E_M - IS$ ($E_\mathrm{B} = E_M + IS$); E_M is a spin-independent chemical potential and IS ($=I \times S$) is the strength of the exchange interaction between a hole and a d spin at the Mn site. On the other hand, a hole is subjected to a spin-independent chemical potential E_A at the Cd site. As long as we regard the d spin at the Mn site as a classical spin, the spin-flip process does not occur in such a strong magnetic field as $\langle S_z\rangle = S$, so the $\uparrow$-spin hole state and the $\downarrow$-spin hole state can

be treated separately. Consequently, this problem agrees with that of the disorder in binary solid solutions. That is, the band-edge energy shift Σ_b for a hole with $\uparrow$ spin ($\downarrow$ spin) is obtained from equation (7) with $E_B = E_M + IS$ ($E_B = E_M - IS$). In figure 1, the result for $IS/\Delta = -0.45$ with $E_M = 0$ as a function of the Mn mole fraction x is depicted by the solid line; $\Sigma_b(+)$ is for $E_{\rm B} = E_M + IS$ and $\Sigma_b(-)$ is for $E_{\rm B} = E_M - IS$.

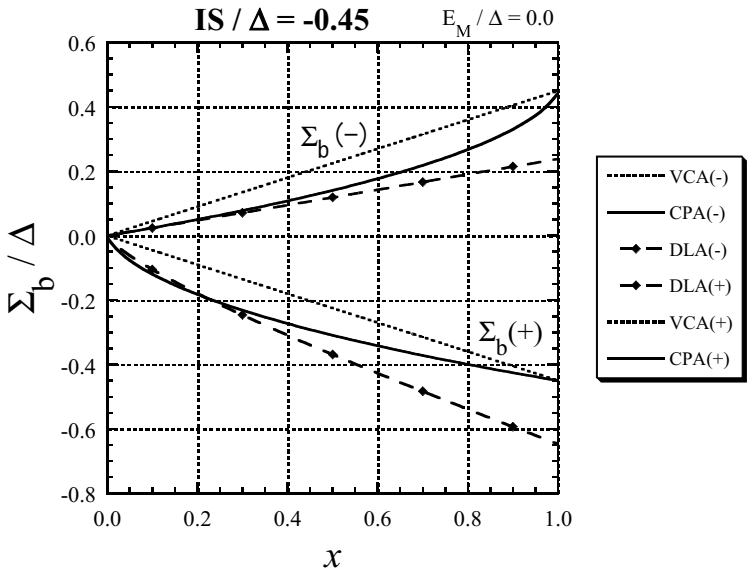

Figure 1. The energy shift of the lowest band edge, Σ_b/Δ, for $IS/\Delta = -0.45$ with $E_M = 0.0$ as a function of the Mn mole fraction x. Solid lines represent the CPA ($\pm$), dashed lines represent the DLA ($\pm$), and dotted lines represent the VCA.

Next, we investigate the VCA and the dilute-limit approximation (DLA) which were previously used by other authors. The VCA gives a result linear in x, namely $\Sigma_b = xE_{\rm B}$ [1,2]. On the other hand, in the DLA, the self-energy is assumed to be x times a t-matrix which describes the multiple scattering on a single B impurity atom in an otherwise regular crystal of A ions ($E_{\rm A} = 0$):

$$\Sigma(\omega) = xt(\omega) = x\frac{E_{\rm B}}{1 - E_{\rm B}F_0(\omega)} = xE_{\rm B}\Big/\left[1 - \frac{2E_{\rm B}}{\Delta}\left\{\frac{\omega}{\Delta} - \sqrt{\left(\frac{\omega}{\Delta}\right)^2 - 1}\right\}\right]. \tag{8}$$

Here, $F_0(\omega)$ is the diagonal matrix element of the Green's function of the host (A-ion) lattice in the Wannier representation, and is equivalent to $F(\omega)$ with $\Sigma \equiv 0$ (see also equation (3)). Substituting $\omega_b = -\Delta + \Sigma(\omega_b)$ into equation (8), we obtain the cubic equation for the energy shift of the lowest band edge, Σ_b ($=\Sigma(\omega_b)$), in the DLA:

$$4\left(\frac{E_{\rm B}}{\Delta}\right)\left(\frac{\Sigma_b}{\Delta}\right)^3 - \left\{4(x+1)\left(\frac{E_{\rm B}}{\Delta}\right)^2 + 4\left(\frac{E_{\rm B}}{\Delta}\right) + 1\right\}\left(\frac{\Sigma_b}{\Delta}\right)^2 + 2x\left(\frac{E_{\rm B}}{\Delta}\right)\left\{2\left(\frac{E_{\rm B}}{\Delta}\right) + 1\right\}\left(\frac{\Sigma_b}{\Delta}\right) - x^2\left(\frac{E_{\rm B}}{\Delta}\right)^2 = 0. \tag{9}$$

For an attractive potential ($E_{\rm B} < 0$), equation (9) gives a real solution of Σ_b (<0). For a repulsive potential ($E_{\rm B} > 0$), however, equation (9) does not give any physical solution. This is because the square root in equation (8) becomes imaginary for $\Sigma_b > 0$ since

$(\omega_b/\Delta)^2 - 1 = (-1 + \Sigma_b/\Delta)^2 - 1 < 0$. Hence, in the DLA [11], for a repulsive potential ($E_B > 0$),

$$\Sigma(\omega_b) = x \operatorname{Re} t(\omega_b) = \operatorname{Re} \frac{xE_B}{1 - E_B F_0(\omega_b)} = \frac{xE_B\{1 - 2(E_B/\Delta)(\omega_b/\Delta)\}}{[1 - (2E_B/\Delta)(\omega_b/\Delta)]^2 + 4(E_B/\Delta)^2\left[1 - (\omega_b/\Delta)^2\right]} \tag{10}$$

is assumed. Combining equation (10) with $\omega_b = -\Delta + \Sigma(\omega_b)$ leads to a quadratic equation for Σ_b ($=\Sigma(\omega_b)$) in the DLA:

$$4\left(\frac{E_B}{\Delta}\right)\left(\frac{\Sigma_b}{\Delta}\right)^2 - \left\{\left(1 + \frac{2E_B}{\Delta}\right)^2 + 2x\left(\frac{E_B}{\Delta}\right)^2\right\}\left(\frac{\Sigma_b}{\Delta}\right) + x\left(\frac{E_B}{\Delta}\right)\left\{1 + 2\left(\frac{E_B}{\Delta}\right)\right\} = 0. \tag{11}$$

It should be noted that different equations are used for Σ_b in the DLA, depending on whether $E_B > 0$ or $E_B < 0$. That is, Σ_b is obtained from equation (9) for $E_B < 0$ and from equation (11) for $E_B > 0$.

In figure 1, the results for the VCA and DLA are included for comparison. The results for the CPA and DLA both equal $\Sigma_b \simeq xE_B\Delta/(\Delta + 2E_B)$ for small x, but begin to separate from each other with increasing x. Figure 1 indicates that when the potential is repulsive ($E_B > 0$), the result for Σ_b from the DLA (equation (11)) is in good agreement with that from the CPA in the range of $x < 0.2$, whereas when the potential is attractive ($E_B < 0$), the separation between the result from the DLA (equation (9)) and that from the CPA begins at $x \sim 0.05$ and becomes very large for $x > 0.3$. When x reaches 1, the results from both the CPA and VCA agree with $\Sigma_b \simeq E_B$, whereas the Σ_b from the DLA takes a value far from E_B; either $E_B < 0$ or $E_B > 0$.

Furthermore, we compare our model with that used by Benoit à la Guillaume *et al* [8] and Tworzydlo [11, 12]. In their model, the square-well potential $U(r) = U\theta(r - b)$ is used with the isotropic effective mass m^* for a carrier; the potential value that marks the appearance of a bound state in the potential well is $U_c = -(\pi\hbar/2b)^2/2m^*$, and the band-edge shift, which is obtained by applying the VCA to their model, is $\Sigma_b = VN_0x = (4\pi b^3U/3)N_0x$. In our treatment, these correspond to $E_B = -0.5\Delta$ (the criterion that a localized level appears) and $\Sigma_b = xE_B$ (the first order of E_B/Δ in equation (7)). For $\Sigma_b(x)$ given by equation (7) in this study, the correction factor due to multiple scattering, $\delta(x) = \Sigma_b(x)/xE_B$, approaches $1/[1 + 2(E_B/\Delta)]$ when $x \to 0$. This agrees with the result obtained previously by other researchers [8, 11, 12] if we assume that $\eta \equiv U/|U_c| = 2E_B/\Delta$ or $(4\pi b^3/3)N_0 = 1$.

The exchange-induced band-splitting energy obtained by applying the VCA to our model is $|2xIS|$, so $[\Sigma_b(+) - \Sigma_b(-)]/2xIS$ exhibits an enhancement in the apparent exchange strength due to the multiple scattering. In figure 2, the present result for $[\Sigma_b(+) - \Sigma_b(-)]/2xIS$ is shown as a function of x for various values of IS/Δ. Figure 2 reveals that the effect of multiple scattering is striking when x approaches zero from 0.2, especially for $|IS/\Delta| > 0.4$. In figure 2, we also include the result from the DLA with $IS/\Delta = -0.45$. At the dilute limit ($x \to 0$), both the CPA and the DLA give the result

$$[\Sigma_b(+) - \Sigma_b(-)]/2xIS = 1/[(1 + 2E_M/\Delta)^2 - (2IS/\Delta)^2].$$

On the other hand, when $x = 1$, the value of $[\Sigma_b(+) - \Sigma_b(-)]/2xIS$ obtained from the CPA is 1. Unexpectedly, the value obtained from the DLA is also almost 1.0 (within 2%), although the values of Σ_b from the DLA are very different from E_B at $x = 1$; either $E_B > 0$ or $E_B < 0$ (see figure 1).

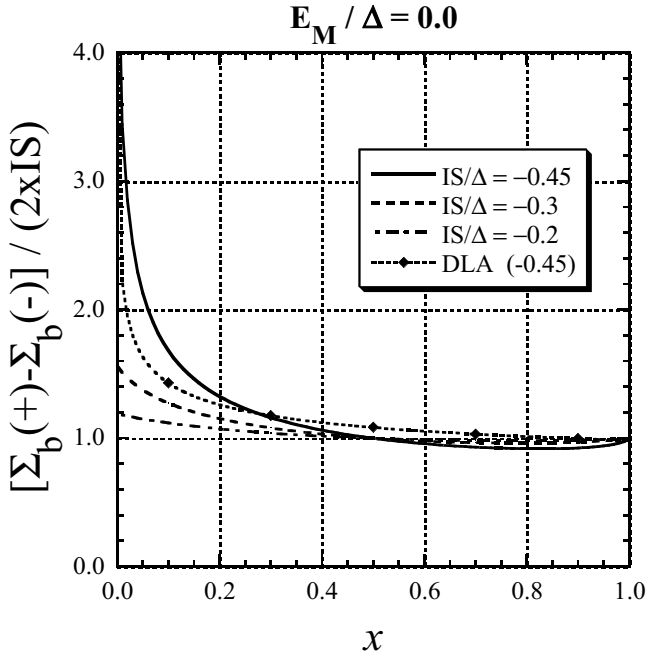

Figure 2. The present results for $[\Sigma_b(+) - \Sigma_b(-)]/2xIS$ with $E_M = 0$, as a function of x ($0 \leqslant x \leqslant 1$), for $IS/\Delta = -0.45$, -0.3, and -0.2. 'DLA' indicates the result calculated using equations (9) and (11) with $IS/\Delta = -0.45$.

The experimentally deduced value of $N_0\beta$ is related to the exchange-induced valence band splitting by $N_0\beta = [\Sigma_b(+) - \Sigma_b(-)]/xS$. In figure 3, we depict the ratio

$$N_0\beta/N_0\beta^* = [\Sigma_b(+) - \Sigma_b(-)]/2xIS$$

as a function of x ($0 \leqslant x \leqslant 0.02$), together with the values of $N_0\beta$ obtained experimentally [4–7] using $N_0\beta^* = -0.72$ eV [13]. Here, $N_0\beta^*$ ($\equiv 2I$) is not an sp exchange integral at $k = 0$ but one averaged over k-space, because point interaction is assumed for the exchange interaction in our model. Comparison between the present result and the experimental observation indicates that the value of $IS/\Delta = -0.45$ (or the bandwidth of $2\Delta = 4$ eV) is suitable for $Cd_{1-x}Mn_xS$. These values are consistent with the best-fitted values used for the explanation of bowing in the energy gap [13].

In order to investigate the E_M-dependence of the exchange band splitting systematically, we show in figure 4 the result for $[\Sigma_b(+) - \Sigma_b(-)]/2xIS$ with $IS/\Delta = -0.40$ as a function of x for various values of E_M/Δ. Note that the impurity band (or localized state) appears at the dilute limit ($x \to 0$) when $E_M/\Delta = -IS/\Delta - 0.5$ (or $E_M/\Delta = -0.1$ for $IS/\Delta = -0.4$). According to Furdyna [1] and Wei and Zunger [9, 10], $(N_0\beta, E_M) = (-1.8$ eV, 0.09 eV) for $Cd_{1-x}Mn_xS$, (-1.11 eV, 0.29 eV) for $Cd_{1-x}Mn_xSe$, (-0.88 eV, 0.44 eV) for $Cd_{1-x}Mn_xTe$, (-1.11 eV, 0.22 eV) for $Zn_{1-x}Mn_xSe$, and (-1.05 eV, 0.53 eV) for $Zn_{1-x}Mn_xTe$. The value of $N_0\beta$ and the width of the sp band in $Cd_{1-x}Mn_xS$ are still controversial [17], while it is certain that the ratio of $|N_0\beta|$ to the bandwidth in $Cd_{1-x}Mn_xS$ is considerably larger than that for other DMSs. In addition, the other DMSs, except $Cd_{1-x}Mn_xS$, have large positive values of E_M. Figure 4 suggests that a positive E_M suppresses the apparent enhancement in $N_0\beta$ for small x in materials other than $Cd_{1-x}Mn_xS$.

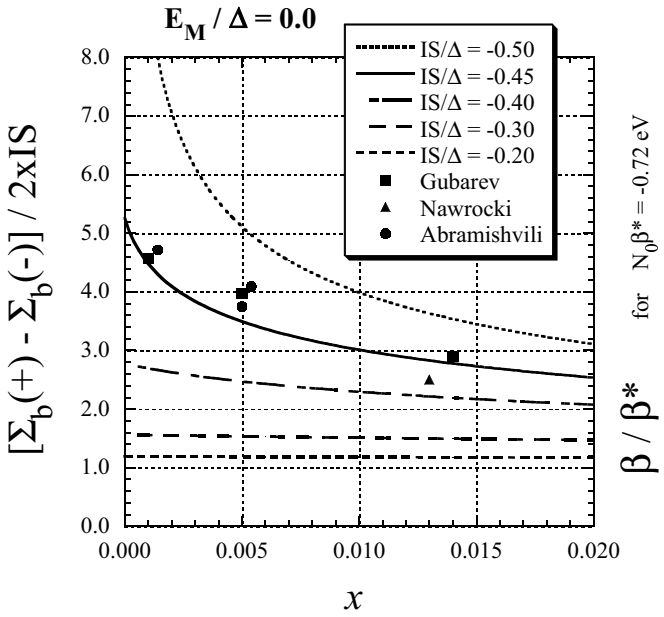

Figure 3. The present results for $[\Sigma_b(+) - \Sigma_b(-)]/2xIS = N_0\beta/N_0\beta^*$ with $E_M = 0$, for $IS/\Delta = -0.45$, -0.30, and -0.2, as functions of x ($0 \leqslant x \leqslant 0.02$). Values of $N_0\beta/N_0\beta^*$ with $N_0\beta^* = -0.72$ eV are included. Experimental data for $N_0\beta$ for $Cd_{1-x}Mn_xS$ are taken from Gubarev and Tyazhlov (reference [4]), Abramishvili and co-workers (references [5] and [6]), and Nawrocki *et al* (reference [7]).

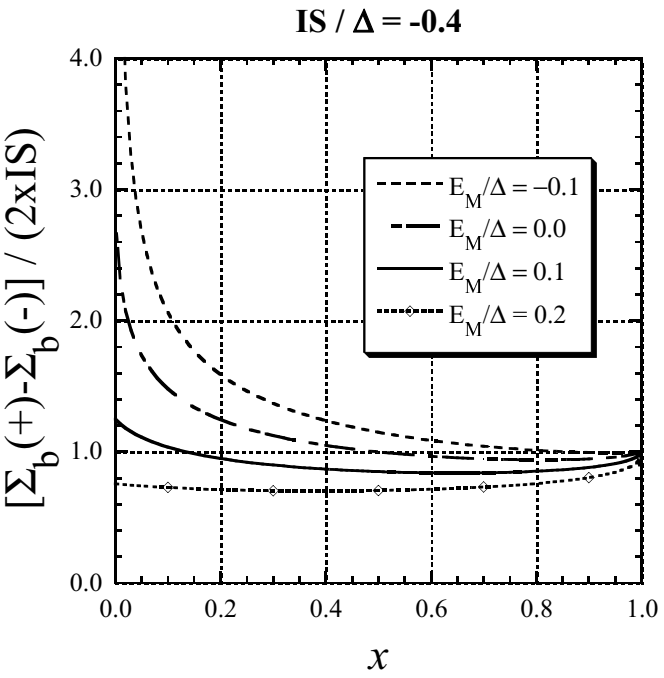

Figure 4. The present results for $[\Sigma_b(+) - \Sigma_b(-)]/2xIS$ with $IS/\Delta = -0.40$, as functions of x ($0 \leqslant x \leqslant 1$), for $E_M/\Delta = -0.1$, 0.0, 0.1, and 0.2.

To summarize, we studied the exchange-induced band splitting in $A^{II}_{1-x}Mn_xB^{VI}$-type diluted magnetic semiconductors (DMSs). When a saturating magnetic field is applied, the previously proposed model [13] agrees with binary solid solutions in which an A ion with local potential E_A and a Mn ion with local potential E_B are distributed randomly with mole fractions x and $1 - x$, respectively; E_B takes the value $E_M - IS$ or $E_M + IS$ according to the spin orientation of the carrier. Applying the coherent potential approximation (CPA) to the model with the undisturbed density of states in the semicircular form, we derived a simple approximate expression for the shift in the lowest band-edge energy (equation (7)), which is applicable over the entire range of x ($0 \leqslant x \leqslant 1$). Next, we investigated the validity of the dilute-limit approximation (DLA). In the DLA the effect of multiple scattering is partially taken into account, while a further inconsistent treatment is required for the calculation of the band edge. That is, different treatments were applied to Σ_b depending on whether $E_B > 0$ or $E_B < 0$, as shown by equations (8)–(11) in this work. Figure 1 suggests that the range of application of the DLA is apparently $x < 0.2$. This makes it possible to use Tworzydlo's theory to explain the abnormal x-dependence of the exchange integral in $Cd_{1-x}Mn_xS$ after fitting some parameters [11, 12]. Throughout this study, in the framework of a simple model with few fitting parameters, we aimed to clarify the effect of the exchange interaction IS and the band-offset energy E_M on the extended carrier state in DMSs. A systematic study linking our method with the valence band-offset parameters obtained by Wei and Zunger [9, 10] revealed the origin of the abnormal x-dependence in $N_0\beta$. The apparent enhancement in the p–d exchange integral ($N_0\beta$) in $Cd_{1-x}Mn_xS$ is a striking manifestation of the multiple-scattering effect which is significant for small x in disordered systems. However, the dominant origin is not a large attractive chemical potential at the Mn site, but a large exchange strength relative to the bandwidth.

Another issue which demonstrates that the VCA with the MFA may not be efficient is the abnormal behaviour at high x reported for $Zn_{1-x}Mn_xTe$ and $Cd_{1-x}Mn_xTe$ [18]; the spin-splitting curves with respect to $|x\langle S_z\rangle|$ are roughly linear, but the slope is significantly reduced at high x-values. Although the CPA becomes inefficient when the clustering or short-range order in the distribution of atoms is appreciable, the above-mentioned observations for $Zn_{1-x}Mn_xTe$ and $Cd_{1-x}Mn_xTe$ may be explained using our model with a positive value of E_M. For a more precise discussion, however, further study on finite values of $\langle S_z\rangle$ is needed. Such calculations are currently under way.

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